

P-tert-Butylthiacalix[4]arenes functionalized by N-(4'-nitrophenyl)acetamide and N,N-diethylacetamide fragments: Synthesis and binding of anionic guests

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Abstract

© 2017 Vavilova and Stoikov; Licensee Beilstein-Institut. New p-tert-butylthiacalix[4]arenes, which are mono-, 1,2-di- and tetrasubstituted at the lower rim containing N-(4'-nitrophenyl)acetamide and N,N-diethylacetamide groups in cone and partial cone conformations have been synthesized. Their complexation ability towards a number of tetrabutylammonium salts $n\text{-Bu}_4\text{NX}$ ($X = \text{F}^-$, Cl^- , Br^- , I^- , CH_3CO_2^- , H_2PO_4^- , NO_3^-) was studied by UV spectroscopy. The effective receptor for the anions studied as well as selective receptors for F^- , CH_3CO_2^- and H_2PO_4^- ions, which based on the synthesized thiacalix[4]arenes, have been obtained. It was shown that p-tertbutylthiacalix[4]arene tetrasubstituted at the lower rim by N-(4'-nitrophenyl)acetamide moieties bonded to the anions studied with association constants within the range of 3.55×10^3 – $7.94 \times 10^5 \text{ M}^{-1}$. Besides, the binding selectivity for F^- , Cl^- , CH_3CO_2^- , and H_2PO_4^- anions against other anions was in the range of 4.1–223.9. Substituting one or two fragments in the macrocycle with N,N-diethylacetamide groups significantly reduces the complexation ability of the receptor. In contrast to the 1,3-disubstituted macrocycle containing two N-(4'-nitrophenyl)acetamide moieties, the 1,2-disubstituted thiacalix[4]arene, which contains only one such fragment and a N,N-diethylacetamide moiety, selectively binds F^- anions.

<http://dx.doi.org/10.3762/bjoc.13.188>

Keywords

Anion binding, Synthesis, Thiacalixarenes, UV spectroscopy

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